

## **National Center for Computational Sciences Snapshot The Week of January 22, 2007**

### **3-D Simulations of Tokamak Plasmas Conducted at ORNL**

Fusion energy research is still in the preliminary stages of theory and simulation, but its potential as a source of clean, virtually unlimited power is slowly being realized at Oak Ridge National Laboratory's (ORNL's) National Center for Computational Sciences (NCCS).

The Gyrokinetic Plasma Simulation team headed by W. W. Lee of the Princeton Plasma Physics Laboratory is using NCCS supercomputers to work toward tapping that potential by exploring turbulence transport, or heat and particle loss, in tokamak reactors.

Tokamaks are doughnut-shaped devices that house the ionized gas responsible for sparking the fusion reaction necessary to produce energy. According to Lee, whose team is simulating turbulent transport on NCCS's Jaguar system, plasmas confined in tokamaks have natural temperature and density gradients that greatly affect the transfer of heat and particles throughout the device. In the core the temperature is hotter and the density higher, while near the walls the temperature gradually becomes cooler and the density lower. These gradients, says Lee, create turbulence, causing significant heat and particle loss in the tokamak.

If the turbulence is too great and the device loses too much heat, the core cannot reach the temperature necessary to ignite a sufficient reaction, sending the entire fusion process into an early demise. Lee's team hopes to create a more consistent environment for ignition reactions by minimizing the effect of the gradients on turbulence and thereby maintaining temperatures in the tokamak.

Lee's project studies two "scaling laws" related to tokamak reactors. The first explores the physical size necessary for a tokamak to achieve ignition. Just as the core must be heated to reach a proper temperature, it likewise must be large enough to facilitate the necessary reactions. Size scaling also helps the researchers determine how confinement can be improved with the application of magnetic fields. According to Lee, a stronger field leads to better confinement, but the relationship is not perfectly understood.

The second investigation involves isotopes and aims to clarify the contradictory theoretical and experimental results surrounding the combination of hydrogen, deuterium, and tritium.

Traditionally, most fusion experiments have used deuterium and hydrogen; but both Lee's simulations and ITER (an upcoming experimental reactor in France that aims to determine the feasibility of fusion power production), as well as several large tokamaks around the world, introduce tritium into the equation.

“Experimental results and theoretical understanding [regarding tritium] don’t agree,” Lee says, adding that while some theories suggest that tritium will weaken confinement and aggravate heat loss, experiments suggest just the opposite. For ITER, and for “real fusion,” as Lee calls it, it is crucial to introduce tritium to achieve a proper reaction. While tritium is radioactive and requires special handling, its half-life of roughly 10 years is much more manageable than that of traditional nuclear waste from fission reactors, which can be upward of 10,000 years.

Lee cites his code’s ability to scale with the Jaguar system as one of its major advantages, adding that it is also capable of scaling well with different machines. Eventually, says Lee, his team hopes to gain access to the planned petascale facilities at the NCCS, which will allow the team to simulate a fusion reactor the size of the proposed ITER facility. The project used 3.5 million processor hours last year, producing successful three-dimensional simulations. In 2007, the project has been awarded 6 million processor hours on the Jaguar system and another 45,000 hours on the Phoenix system through the Department of Energy program Innovative and Novel Computational Impact on Theory and Experiment (INCITE). Lee calls the computing power available at the NCCS “crucial” to his team’s research and emphasizes the importance of continuing the fruitful interactions with members of ORNL’s Scientific Computing Group.

“Dr. Scott Klasky of NCCS is a co-principal investigator of our SciDAC [Scientific Discovery through Advanced Computing] project, and he serves as a crucial link for us in accessing these resources,” says Lee. “We want them to provide us with the fastest and most powerful computers available and the most advanced software tools. We are on our way.”

### **Training Explores the Inner Workings of Lustre**

More than 30 systems experts gathered at the NCCS last week to get a highly detailed look at the high-performance Lustre file system.

The Lustre Internals Training, provided as part of the Lustre Centre of Excellence housed at the NCCS, was held January 17–19. Lustre is a highly scalable file system used on some of the world’s fastest supercomputers, including the Jaguar system at the NCCS.

The training was conducted by Peter Braam, chief technology officer of Cluster File Systems, Inc., and Lustre’s primary architect.

“I thought it went well,” said NCCS Technology Group leader Shane Canon. “We learned a lot of good details about how to troubleshoot problems, how to gather and analyze logs, and where certain metrics can be gathered to see how the system behaves.”

The class provided information on the Lustre architecture. It also provided an in-depth look at how the system handles a variety of tasks, ways of analyzing it at each layer, and strategies for troubleshooting.

Although the latest class was primarily for systems experts, future training will focus on helping application developers make the best possible use of the Lustre system.

### **NCCS Users to Gather in March**

NCCS users will gather at ORNL for a 3-day meeting in March to ensure that they make the most of their allocations on the center's world-class supercomputers.

The 2007 NCCS User Meeting, scheduled for March 27–29 at the Joint Institute for Computational Sciences building at ORNL, will feature presentations and tutorials on a range of topics, from closeup looks at system architecture to an overview of solutions for data storage. Representatives have been invited from the 28 projects that will be using the systems through the Department of Energy's INCITE program.

These users have been allocated more than 75 million processor hours on the Cray XT4 Jaguar system and the Cray X1E Phoenix system. These systems will be providing more than three-quarters of the computing power allocated for the INCITE program, paving the way for breakthrough discoveries in chemistry, biology, fusion science, climate science, materials science, astrophysics, and other critical fields.

Topics for the meeting include system administration issues relevant to users, system architecture and software, scientific visualization, data analysis, and Cray's plans for the future. Tutorials will be available that focus on the Cray XT4 and X1E, visualization, and Cray performance tools.

The event will also host a series of user presentations and a user meeting that will give scientists an opportunity to discuss the challenges they face in using these state-of-the-art systems.